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Chapter 2 - Quantum Phase Transitions

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Abstract

Quantum phase transition (QPT) occurs at zero temperature where thermal fluctuations are absent and instead the transition is driven by quantum fluctuations which are tuned by variations in some nonthermal parameters, such as pressure, magnetic field, or chemical composition, as demanded by Heisenberg's uncertainty principle. Although QPT occurs at zero temperature, its influence expands to a broad nonzero temperature regime of quantum criticality, enabling us to study these phenomena through variety of experimental techniques. This chapter considers QPTs in quantum magnets, presenting a brief introduction to several well-studied systems and reviewing experimental examples for spin dimers, geometrically frustrated magnets, heavy fermions, itinerant magnets, and transverse field Ising systems, with focus on neutron scattering techniques utilized to deliver a more comprehensive picture of the fundamental physics behind the QPT in these systems.

Introduction

The distinguishing characteristic of a phase transition is the sudden change in one or

more physical properties. Studies of quantum magnetism consider systems in which the effects of quantum fluctuations, as well as thermal fluctuations, must be considered. Our most familiar conception of a phase transitions is that driven by fluctuations caused by tuning the temperature close to some critical value T_c, known as a classical phase transition (CPT). As the sample temperature is raised above T_c, thermal fluctuations, whose scale is controlled by k_BT where k_B is the Boltzmann constant, destroy the order and drive the system across the phase transition. Conversely, thermal fluctuations decrease as the temperature is dropped and eventually freeze out as $T \rightarrow 0$. Quantum fluctuations, on the other hand, continue to live on at zero temperature and thus, under certain conditions, trigger the system to encounter a phase transition between different quantum phases at $T=0$. This transition at zero temperature is known as a quantum phase transition (QPT), where the underlying quantum fluctuations are determined by Heisenberg's uncertainty principle. The amplitude of these quantum fluctuations can be tuned by varying an external parameter in the Hamiltonian governing the system, such as applied magnetic field, pressure, or doping level of chemical, which eventually results in development of a new preferable lower-energy ground state.

The degree of ordering in a system is the outcome of competition between interactions that enforce ordering to minimize internal energy and thermal fluctuations that increase disorder to maximize entropy. For many systems this results in the formation of different macroscopic phases. The transformation of a system from one of its phases into another is referred to as a CPT. A CPT happens when the free energy of the system or one of its derivatives is discontinuous. The transitions between solid, liquid, and gaseous phases of water, or the transition between the ferromagnetic and paramagnetic (PM) phases of magnetic materials at the Curie point, are familiar examples of such transitions. For detailed discussions on phase transitions, see Refs [1], [2].

According to the modern classification, phase transitions are divided into two broad categories: first-order or discontinuous transitions and second-order or continuous transitions.

If there is a finite discontinuity in one or more of the first derivatives of the appropriate thermodynamic potential, the transition is first-order or discontinuous. For example, this can be a discontinuity in the magnetization in a magnetic system. Figure1 illustrates neutron diffraction data collected at the 1/2 (0,1,3) Bragg reflection of $KMnF_3$, exhibiting temperature dependence typical of a first-order phase transition. An additional characteristic of first-order phase transitions is the existence of latent heat. This means that during such a transition the system either absorbs or releases a fixed amount of

energy and, since energy cannot be instantaneously transferred between the system and its environment, first-order transitions are associated with “mixed-phase regimes” in which some parts of the system have completed the transition and others have not. A good example is freezing of water during which the temperature remains constant as the heat is transferred into the environment and the system remains in a mixed phase of fluid and solid until the entire structure has transitioned.

The second class of phase transitions is second-order or continuous phase transitions. These are the transitions in which the first derivatives of thermodynamic potentials are continuous but the second derivatives are discontinuous or infinite. Figure2 shows the temperature-dependent behavior of neutron diffraction measurements of NbO_2 collected at the superlattice reflection (5/4,5/4,3/2), demonstrating neither discontinuity nor any hysteresis in the intensity, thus signifying the second-order nature of the semiconducting-to-metallic phase transition. The key feature of second-order or continuous phase transitions is the existence of fluctuating microregions of both phases near the critical point. The characteristic length of these fluctuating regions diverges at the critical point. For further discussions on neutron scattering techniques used to study the critical phenomena, see Ref.[5].

A continuous phase transition can be characterized by an order parameter, a thermodynamic quantity that is zero in one phase (disordered) but has a finite value in another phase (ordered). For instance, in a ferromagnetic phase transition, the total magnetization is an order parameter.

Although the thermodynamic average of an order parameter is zero in the disordered phase, its fluctuations are nonzero. The spatial correlations of the order parameter fluctuations become long-ranged, as the system approaches the critical point at which it goes through the phase transition; eventually the typical length scale of the order parameter fluctuations, known as the correlation length ξ, diverges as:$\xi \propto |t|^{-\nu}$where t is some dimensionless measure of the distance from the critical point (in the case where the transition occurs at a nonzero temperature T_c, t equals $|T-T_c|/T_c$) and ν is the correlation length critical exponent [6].

Since the correlation length is the only relevant length scale near the critical point, if one rescales all lengths in the system by an arbitrary factor b while simultaneously adjusting the external tuning parameter x such that the correlation length maintains its initial value, the physical properties of a system should remain unchanged. This is known as the homogenous form of the free-energy density f near the critical point:

$f(t,x) = b^{-d} f\left(tb^{\frac{1}{\nu}}, xb^{y_x}\right)$ where d is the space dimensionality, y_x is critical exponent associated with the external tuning parameter x, which, for example, could be external magnetic field or pressure (for in-depth discussions, see Refs [7], [8], [9], [10]).

Other thermodynamic quantities can also be extracted by differentiating the free energy, giving rise to various critical exponents. Common critical exponents used in magnetism are shown in Table 1.

However, not all exponents are independent from each other [11], [12]. The scaling relations shown in Eqn (3) link the four thermodynamic exponents α, β, γ, δ.

$$2-\alpha = 2\beta+\gamma = \beta(\delta+1) 2-\alpha = d\nu\gamma = (2-\eta)\nu$$

(4), (5) are referred to as hyperscaling relations. Equation (4), which is also known as Josephson's identity, is only valid for system dimension $d \leq 4$. In continuous QPTs, critical exponents are the same for all classes of phase transitions which may occur in various physical systems based on their system dimension. This remarkable feature is known as universality [9], [13].

Continuous phase transitions at $T=0$ are called QPTs, where thermal fluctuations have vanished and quantum fluctuations demanded by Heisenberg's uncertainty dominate. In continuous phase transitions, depending on the values of the external tuning parameters, the order parameter either is zero or has a finite value and a variation of external parameters can switch the order parameter on or off in the ground state of the system. At finite temperature a phase transition is driven by thermal fluctuations, whereas in QPT at $T=0$ some other nonthermal external parameters such as pressure, magnetic field, or chemical doping tune the quantum fluctuations of the system and thus drive it into the phase transition. In this case the corresponding density operator $\mathbf{e}^{-\beta\mathcal{H}}$ resembles a time evolution operator $\mathbf{e}^{-i\tau\mathcal{H}}$, where $\tau \equiv -i\beta$ and $\beta = 1/k_B T$, and accordingly shows a fundamental difference between CPT and QPT: in QPT not only the correlation length in the spatial dimension d diverges when $T \to 0$ but also the correlation along the direction of imaginary time $i\tau = 1/k_B T$ extends to infinity as the temperature goes to zero [14]. Thus at zero temperature the imaginary time acts as an additional dimension, and the homogeneity law for the free-energy density can be rewritten as:

$f(t,x) = b^{-(d+z)} f\left(tb^{\frac{1}{\nu}}, xb^{y_x}\right)$ where z is referred to as the dynamic critical exponent. In general, z may be different from 1 since the length scales in space can be different from the length scale in the imaginary time direction. Comparing Eqn (6) to the homogeneity law obtained for CPT, it is concluded that all the scaling forms are very similar,

considering that a QPT in spatial dimension d is equivalent to a CPT in spatial dimension $d+z$. As a result, the hyperscaling relation for QPT is modified as:$\boldsymbol{2-\alpha=(d+z)\nu}$

As system temperature approaches T=0, thermal fluctuations reduce, and consequently quantum fluctuations become more dominant. Although it is not possible to observe a system at T=0, it is conceivable to reach low enough temperatures where quantum fluctuations are more prominent than thermal fluctuations. Similar to Eqn (1), the correlation length along the imaginary time dimension is given as:$\boldsymbol{\xi_\tau \propto |t|^{-\nu z}}$ and thus as T approaches zero and the correlation length along spatial dimensions diverges, so does the correlation length along the imaginary time dimension.

The quantum critical point (QCP) is the point where the system goes through the QPT at zero temperature. Although the QPT occurs at T=0, its effects can be observable in the vicinity of the QCP. The system behavior near QCP is the result of competing thermal fluctuations, as a function of thermal energy scale k_BT, and quantum fluctuations, as a function of quantum energy scale $\boldsymbol{\hbar\omega}$. The crossover between classical and quantum behavior occurs when the correlation time reaches $1/k_BT$. Since the correlation time, the shortest time allowed by the quantum mechanics for the system to return to equilibrium after an external arbitrary perturbation, is finite, the crossover temperature is nonzero. This allows for the experimental observation of nonthermally induced QPT behavior at a small but nonzero temperature below the crossover temperature [15].

In the vicinity of QCP at x=x_c, where x_c represents the critical value of the tuning parameter at QPT, at lengths smaller than ξ, the ground state wave function has an entangled critical form, whereas it has a noncritical form atlonger lengths. Furthermore, at finite temperatures, the system has an additional characteristic length $\boldsymbol{\hbar\omega/k_BT}$, the so-called de Broglie wavelength of excitations at x_c. For $\boldsymbol{\xi<\hbar\omega/k_BT}$ the ground state wave function has a noncritical form where thermal fluctuations are suppressed. In this case the ground state is thermally excited as temperature rises. For $\boldsymbol{\xi>\hbar\omega/k_BT}$, however, the wave function is in quantum critical region, and thermal fluctuations act directly on the quantum entangled ground state.

There are two types of phase diagrams: with or without a long-range ordered phase at finite temperatures. These phase diagrams are shown in Figure3 as function of temperature versus tuning parameter x. Upon rising temperature the thermal fluctuations destroy the ordering as the system crosses the phase boundary. As x increases, the quantum fluctuations become more important, and the system will be in a quantum disordered state. If a long-range ordered phase at finite temperature exists (as

shown in the left panel of Figure 3), the system will become ordered at low enough temperatures depending on the magnitude of tuning parameter x. At higher temperature the long-range order will be destroyed by thermal fluctuations. By varying the tuning parameters x (magnetic field, pressure, or chemical doping) at low enough temperature, one can observe a crossover from the classical region into the quantum critical region in the quantum disordered phase. If no long-range ordered phase exists in the system at finite temperature as shown in the right panel of Figure 3, one will not see an actual phase transition in the experiment, but instead a sharp crossover as the system passes the quantum critical region, turning more prominent as the temperature approaches zero, and the system gets closer to the QCP.

The fan shape region in the middle of the phase diagrams shows the quantum critical region, where the thermal and quantum fluctuations are of the same order of magnitude and are both important. The region has a characteristic fan shape corresponding to the fact that ξ diverges as $x \rightarrow x_c$. Thus surprisingly with increasing temperature, the influence of the quantum criticality (QC) also increases and even expands beyond the QCP at $T=0$. Describing the dynamics of the complex critical state and developing a theory that explains QC has been the subject of intensive theoretical and experimental research. For a comprehensive discussion on QPT, see Ref. [14].

Section snippets

Experimental Techniques

Systems exhibiting QPTs are expected to show unusual dynamics controlled by external parameters such as applied magnetic fields, pressure, and chemical doping that tune the quantum fluctuations. The exotic characteristic of these systems can be probed with neutron scattering techniques under extreme environmental conditions. In this section, we briefly review the key aspects of neutron scattering methods typically used to investigate quantum magnetic systems. In the following section, we …

Extreme Environmental Conditions

Systems exhibiting QPTs are expected to show unusual dynamics controlled by external parameters, such as applied magnetic fields, pressure, and chemical doping, which tune

the quantum fluctuations and can be probed with neutron scattering techniques under extreme environmental conditions. The three most common neutron scattering extreme environmental conditions employed to study magnetic systems are cryogenic temperatures, high magnetic fields, and pressure. As discussed in earlier sections, …

Spin Dimer Systems

Along with mass and charge, spin is one of the fundamental properties of elementary particles. Interactions between particle spins and the interplay between spin and charge give rise to a rich variety of collective phenomena, making spin materials a fruitful laboratory for studying the onset of ordering, dimensional crossovers, and other questions related to QPTs. Novel collective quantum phenomena were recently observed in magnetic spin dimer systems. Magnetism in these systems consists of …

XY Pyrochlore Magnets

Pyrochlore magnets have been a playground for the physics of geometrical frustration as the A-site of cubic pyrochlores of the form $A_2B_2O_7$ form a network of corner-sharing tetrahedra, shown in Figure36 [80]. The family of rare earth titanates, $R_2B_2O_7$, has been of particular interest, as a range of R^{3+} ions can occupy the A-site, and the B-site of the pyrochlore structure is occupied by nonmagnetic Ti^{4+} [81].

As rare earth ions reside at the bottom of the periodic table, where spin–orbit …

Heavy Fermions

Discovery of heavy-fermion and cuprate superconductivity in the 1980s has generated significant interest in the field of strongly correlated electron materials. In forefront of research in this field are efforts to establish how electrons are organized and to ascertain whether there are universal principles that control various classes of these materials. One such principle is QC [96] which facilitates a continuous phase transition at absolute zero temperature between distinct ground states of …

Weak Itinerant Ferromagnets

Although there is clear evidence for AF QCPs, the existence of an FM QCP still remains an open question. Recent substantial experimental and theoretical efforts have indicated

that depending on the strength of quenched disorder, the ferromagnetic quantum transitions can be classified in different categories [122]. For pure systems, there is a discontinuous, or first-order, QPT from the ferromagnetic to a PM ground state as a function of the control parameter (hydrostatic pressure or uniaxial …

Transverse Field Quantum Ising Model

Although the underlying physics of QPTs are complex and challenging, there are few relatively simple models which can demonstrate the fundamentals of this rich phenomena. Among them, Ising magnet in a transverse external magnetic field is the simplest quantum spin model. Choosing the z-axis to be the Ising axis, the corresponding Hamiltonian is given by:$\boldsymbol{H = -\sum_{\langle ij \rangle} J_{ij}^{zz} S_i^z S_j^z + \Gamma \sum_i S_i^x}$ where $\boldsymbol{S_i^z}$ and $\boldsymbol{S_i^x}$ are the z and x components of the spin at lattice site i, respectively. $\boldsymbol{J_{ij}^{zz} > 0}$ is the longitudinal …

Closing Remarks

The variation of external parameters changes the characteristics of a system, resulting in phase transitions. We encounter with phase transitions in our dailylives: the thermal motion of water molecules destroys the crystal structure of the ice, as it melts and transits into the liquid phase. In thermal phase transitions the order, which exists at lower temperatures, is destroyed by thermal fluctuations. QPTs, however, occur at zero temperature where thermal fluctuations are fully suppressed, …

Acknowledgments

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> ...In these cases, the structural transition temperature TS remains coincident with the magnetic transition temperature TN, and superconductivity is induced for ~20% dopants. BaFe2(As1−xPx)2 is especially interesting because of the numerous reports of a quantum critical point [140] in this system [141]. However, results from single-crystal neutron diffraction suggest magnetic order in this system also disappears in a weakly first-order fashion [142]....

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